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In-situ Raman and PL spectroscopy of phosphorene under highpressure¹ MEYSAM AKHTAR, SAHAR PISHGAR, GAMINI SUMANESEKRA, Univ of Louisville, JACEK JASINSKI, Conn Center for Renewable Energy Research — Few-layer black phosphorus (phosphorene), a novel two-dimensional (2D) material is gaining attention, particularly for electronic applications, because of high carrier mobility ($^{10^3}$ cm²V⁻¹s⁻¹) and a direct, layer number-dependent bandgap, changing from 0.3 eV for bulk to ~2 eV for a monolayer BP. Several recent theoretical studies have indicated that strain engineering can be a viable strategy to additionally tune the electronic structure of phosphorene. Reversible direct-indirect bandgap and semiconductor-metal transitions have been predicted under compression strain for monolayer as well as few-layer phosphorene. Here, we conducted a systematic experimental study of these phenomena, by in situ high-pressure Raman and PL spectroscopy. Few-layer black phosphorus (phosphorene) samples, with varying sizes and number of layers, was prepared by liquid exfoliation, a diamond anvil cell (DAC) was used to create high-pressure conditions (up to ~15 GPa), and in situ, optical spectra were measured using a micro-Raman/PL system. The experiment accompanied with theoretical calculations of vibrational modes to a better understanding of high-pressure effects on optical properties and band structure of this material system.

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